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Automatic TCAD calibration based on Bayesian optimization for SiC MOSFET

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Silicon carbide (SiC) is critical for high-temperature and radiation-hardened power applications [1]. For SiC device design, technology computer aided design (TCAD) is an indispensable tool. Nevertheless, default TCAD physical models produce large discrepancies between simulation and measurement. The calibration process is highly complex due to the large number of coupled physical parameters belonging to various models [2]. Even though machine learning algorithms have been adopted, state-of-the-art work still demands ∼1000 simulations [3]. To boost calibration efficiency, this study proposes a fully automated SiC TCAD calibration workflow integrating multi-objective Gaussian process (MOGP) and Bayesian optimization (BO), achieving below-2% max normalized root mean square error (max NRMSE, i.e., the largest NRMSE among the target I-V curves) for three transfer and output characteristics within only ∼250 simulations (Figure 1(a)). The strategy provides a generalized tool for semiconductor TCAD calibration.

Device and simulation setup. Figures 1(b) and (c) show the cross-section and focused ion beam (FIB) image of the investigated SiC MOSFET, fabricated on an N-epi/N-sub wafer with a 2 μm channel length, 60 μm channel width, and 45 nm gate oxide. Detailed fabrication process conditions are provided in Appendix A. Under identical structure and process conditions, the device is simulated in Sentaurus TCAD 2024 with four mobility models activated (DD, EL, EIC, and HFS) and fixed positive charges added at the SiC/SiO_2 interface to emulate the poor interface quality; detailed model descriptions are provided in Appendix B. Figures 1(d) and (e) show the simulated I-V curves under initial (typical) model parameters alongside measurements, yielding NRMSE values of 141.8%, 57.1%, and 36.5% for the output curve at $V_{GS} = 10$ V, output curve at $V_{GS} = 20$ V, and transfer curve at $V_{DS} = 20$ V, respectively, confirming the necessity of calibration.

Calibration workflow. Figure 1(a) illustrates the complete workflow. The calibration selects 14 TCAD model parameters involving the mobility models and interface states, with their physical interpretations and search bounds listed in Appendix B. An initial set of 100 simulations is generated by Latin hypercube sampling (LHS) to uniformly cover the parameter space. Principal component analysis (PCA) is applied to reduce the dimensionality of the I-V calibration curves, upon which a MOGP surrogate model is established [4]: for a given set of TCAD model parameters, the MOGP predicts the corresponding I-V curves together with prediction uncertainty, making it a well-suited surrogate for BO. BO then proposes three distance-penalized candidate points per iteration [5]. Based on these candidates, the TCAD is rerun to generate new results to update the MOGP surrogate model, and the loop repeats until the max NRMSE falls below the 2% convergence threshold. The detailed algorithmic procedure and pseudocode are provided in Appendix C.

Results and discussion. Among the 100 initial LHS simulations, the best sample still yields a max NRMSE above 15%, confirming that exhaustive parameter search is insufficient. Figure 1(f) illustrates the state of the MOGP model at the first BO iteration. The candidate proposed by BO is expected to closely approach the calibration target according to the MOGP prediction, yet the confidence interval is very wide ($R^2 \approx 0.65$), reflecting limited model fidelity at this early stage. The actual TCAD simulation at the BO-proposed parameter set deviates noticeably from the target, since BO deliberately explores uncertain regions of the parameter space rather than exploiting the current best. Figures 1(g) and (h) show the evolution of R^2 and max NRMSE over BO iterations: by the 50th iteration (150 additional simulations), R^2 exceeds 0.95, and the max NRMSE drops below 2%. Figures 1(i) and (j) show that the final calibrated I_D-V_{DS} and I_D-V_{GS} curves agree well with measurement for all three targets. Including the initial dataset, the entire workflow requires only ∼250 TCAD simulations, achieving significantly improved sample efficiency over

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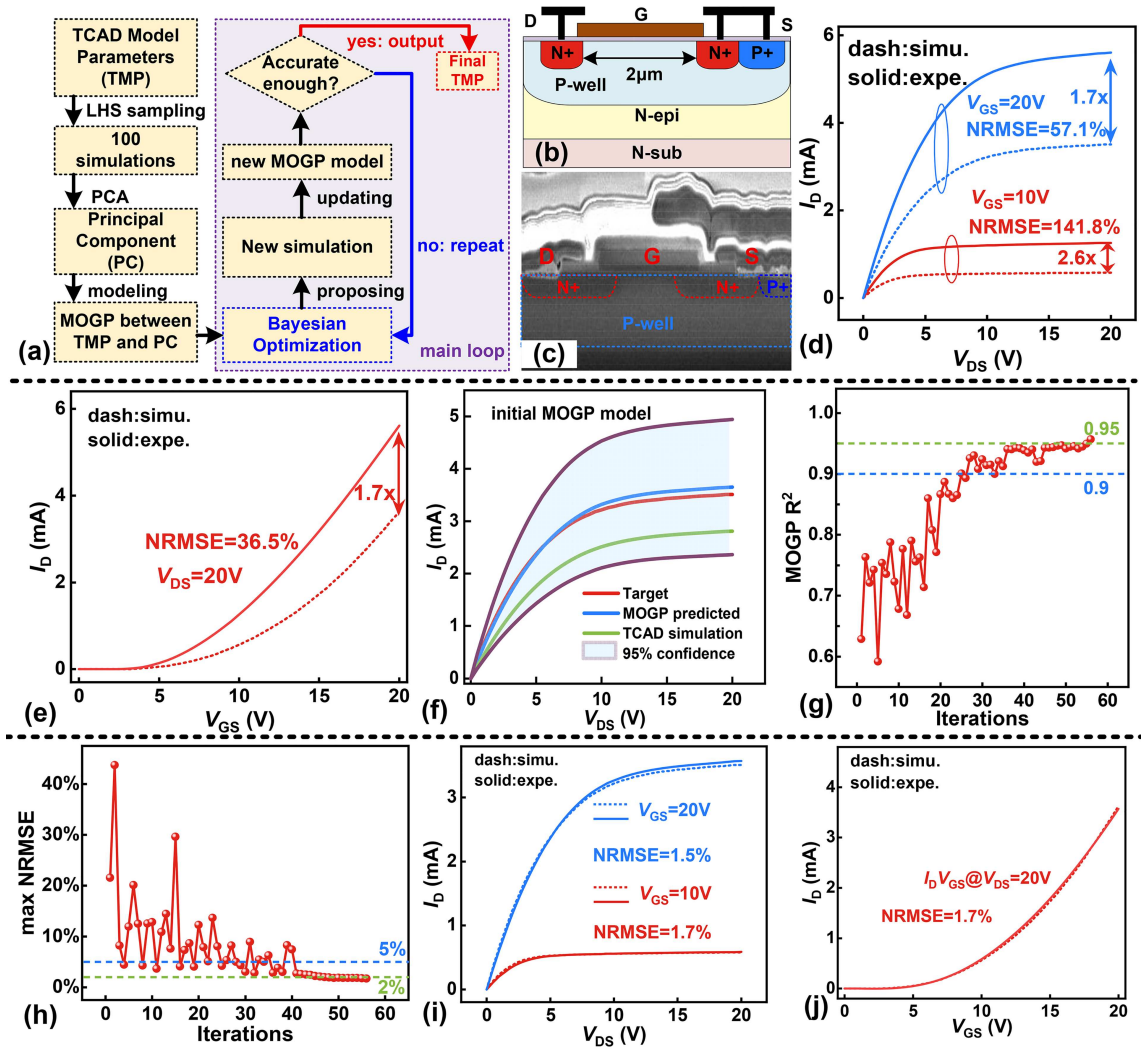

Figure 1 (Color online) (a) Proposed automated TCAD calibration workflow. (b) Schematic and (c) FIB cross-sectional image of the SiC NMOS device. Comparison of *I-V* curves between initial TCAD simulation and measurement: (d) output characteristics and (e) transfer characteristic. (f) Comparison of target, MOGP-predicted, and TCAD-simulated curves at the first BO iteration. Evolution of (g) surrogate model accuracy R^2 and (h) max NRMSE (the largest NRMSE among the three target *I-V* curves) over BO iterations. Comparison of *I-V* curves between calibrated simulation and measurement: (i) output characteristics and (j) transfer characteristic.

recent automated calibration methods [3]. The final calibrated parameter values and benchmark against other reported methods are listed in Appendixes B and D, respectively.

Conclusion. A sample-efficient automated TCAD calibration workflow for SiC devices is proposed by integrating PCA, MOGP, and BO. Using only ∼250 TCAD simulations, the workflow achieves below-2% max NRMSE for transfer and output characteristics, representing a significant improvement in simulation efficiency over existing automated methods.

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Supporting information Appendixes A–D. The supporting information is available online at info.scichina.com and link.springer.com. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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